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Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 136 °C

Global applicability domain: Inside

Local applicability domain index: 3.51e-01

Confidence level: 7.06e-01

Nearest Neighbors from the Training Set

Image not found

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Measured: 136
Predicted: 136

Image not found

Lomustine Measured: 89.0 Predicted: 97.7 Image not found

Isocil

Measured: 159 Predicted: 158

Image not found

Bromacil Measured: 158 Predicted: 157 Image not found

Tranid

Measured: 144 Predicted: 141